Direct Methods for Surface Crystallography

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Due to differences in their environments compared to their counterparts in the bulk of a material, atoms near a surface take on unusual arrangements. A determination of these structures by the techniques of surface crystallography is the key to understanding many important phenomena, such as catalysis and corrosion, and the growth of novel materials. The direct determination of surface structures by e.g. x-ray diffraction is hampered the fact that the phases of the scattered radiation are not measured. We have proposed and demonstrated a solution to this *phase problem* of surface crystallography

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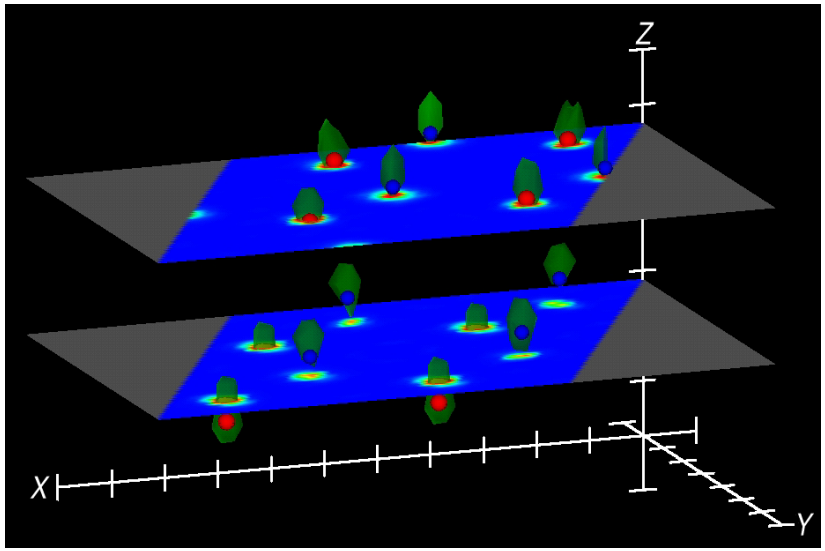

Isosurfaces of electron density of the upper two bilayers of the "vacancy buckling model of the GaAs(111)-(2x2) surface recovered directly from simulated surface x-ray diffraction data by an iterative phasing algorithm. The red spheres mark the positions of the As atoms, and the blue ones those of Ga.

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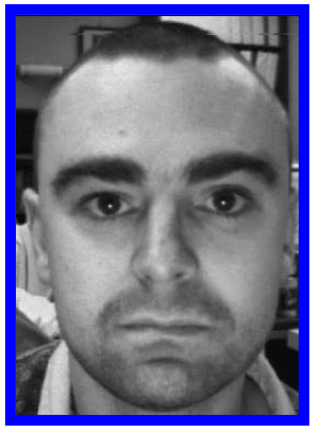
Education:

An undergraduate student, Zao Wang, contributed to this work as part of the UWM Physics Department's NSF-funded Research Experiences for Undergraduates program. Other contributors were graduate students, Ross Harder and Mark Pauli, who received their Ph.D.s in 2002, as well as a current graduate student, Russell Fung. Harder took up a post-doc position at the University of Illinois, and Pauli joined a California company specializing in image processing. Pauli and Fung have both been recipients of competitive UWM Graduate School Fellowships.

Mark Pauli
Ph.D. 2002

Joined California scientific programming company



Ross Harder
Ph.D. 2002

Post-doc University of Illinois at Urbana-Champaign